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14. ABSTRACT

For several years, we have been accurately calculating the electronic structure of superlattices using a solution technique based on the Empirical Pseudopotential Method (EOM). In our method for forming the superlattice pseudopotential, the critical assumption is that the heterointerface charges are redistributed, making each constituent layer in the superlattice as bulk-like as possible. Here, we demonstrate that our technique for forming the superlattice pseudopotential is fundamentally different from the atomistic pseudopotential approaches that use a superposition of atomic pseudopotentials to represent the superlattice. We then present several applications of our method to InAsGaSb Type-II superlattices and, where possible, we compare our results to those calculated with an effective mass method, as well as to atomistic EPM methods. In all of these comparisons, our method provides excellent agreement with the measured data.

15. SUBJECT TERMS

Empirical Pseudopotential, superlattice, InAs, GaSb, type II interface

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Empirical Pseudopotential Modeling of Superlattices

AS AMENDED DEO-PA

Gregory C. Dente, Michael Tilton, Andrew Ongstad

INSERT→ Air Force Research Laboratory Directed Energy Directorate

" Standard Model "

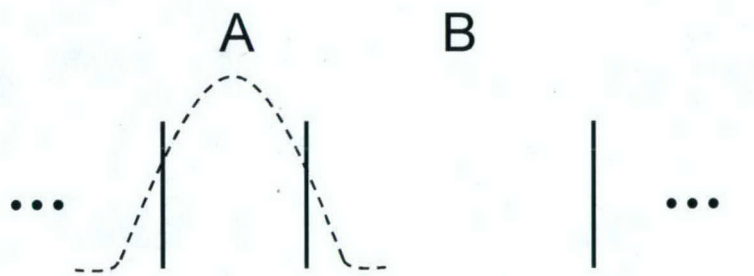
$\vec{k} \cdot \vec{P}$ perturbation theory

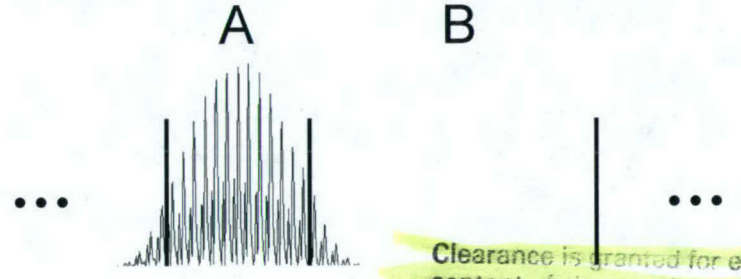
+

Envelope Function Approximation

More Exact Models (EPM)

Solve the Schroedinger Eqn. for a more microscopically correct potential:





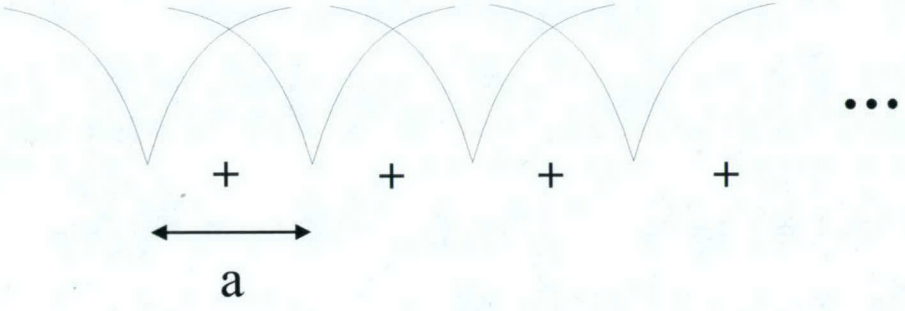
- We will concentrate on the EPM based models:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi = E\Psi$$

Physics of Bulk Solids with EPM

- Constructing the bulk potential:

$V(\vec{r}) =$



$$V(\vec{r}) = \sum_{\vec{t}} \Omega_{\substack{lattice \\ site}}(\vec{r}+\vec{t}) \overset{\text{Poisson Sum Formula}}{=\!=} \sum_{\vec{g}} V_{\vec{g}}\, e^{i\vec{g}\cdot\vec{r}} \qquad V_{\vec{g}} \;\alpha\; \tilde{\Omega}(\vec{k})\Big|_{\vec{k}=\vec{g}} = \textit{form factor}$$

in which $\{\vec{g}\}$ are the reciprocal lattice vectors such that $\vec{g}\cdot\vec{t} = \text{Integer}\cdot 2\pi$.

This forces:

$$V(\vec{r}) = V(\vec{r}+\vec{t})$$

$$\left(\frac{\hbar^2}{2m}\left|\vec{\xi}+\vec{g}\right|^2 + V_0 - E(\vec{\xi})\right) b_{\vec{g}}(\vec{\xi}) + \sum_{\vec{h}} V_{\vec{g}-\vec{h}}\, b_{\vec{h}}(\vec{\xi}) = 0$$

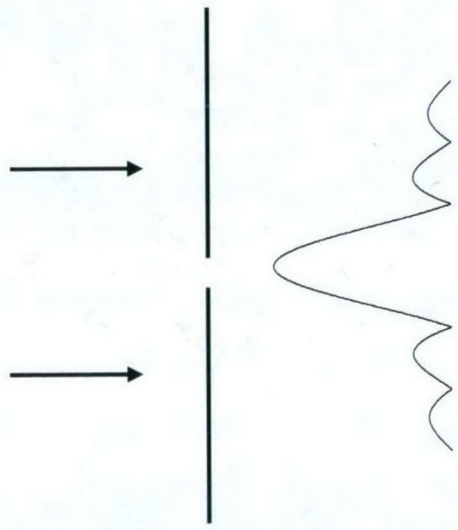
Key Point

- We do not need to know the full lattice potential:

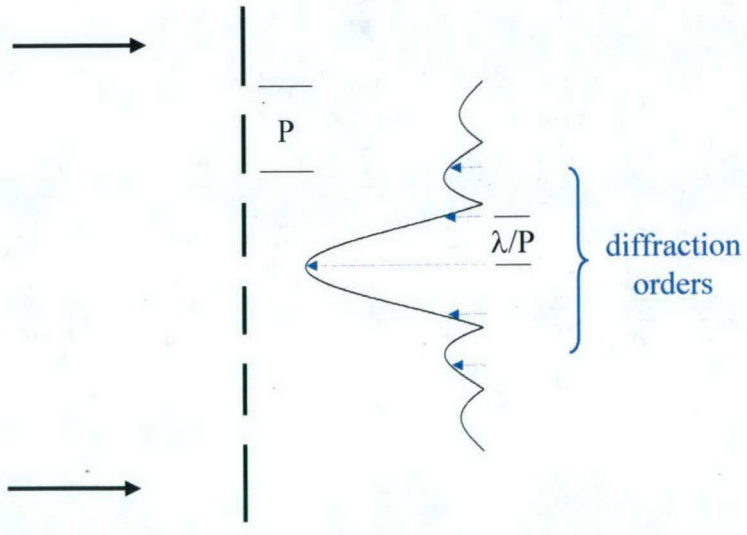
$$\textit{Fourier Transform}\{\,\Omega(\vec{r})\,\} \equiv V(\vec{k}) \qquad -Max < k_x, k_y, k_z < Max$$

We only need $V(\vec{k} = \vec{g}) \equiv V_{\vec{g}}$ *(form factors)*

Optics Analogy:



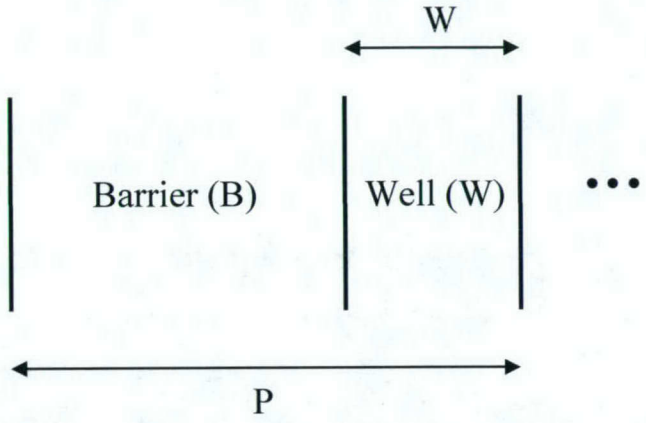
Single Slit



Array of Slits

How do we form V for the Superlattice ??

- There are at least two methods for representing the potential of a superlattice (W / B):



- Method (1) : "Atomistic" EPM = AEPM

$$V(\vec{r}) = \sum_{\text{Sum over W-sites}} \Omega_W(\vec{r}+\vec{t}_W) + \sum_{\text{Sum over B-sites}} \Omega_B(\vec{r}+\vec{t}_B) + \textit{Interface detail}$$

Key Point: This construction requires functional fits to $\Omega_W(\vec{r})$ *and* $\Omega_B(\vec{r})$ + *others*

Example: InAs / GaSb requires $\Omega_{In(As)}(\vec{r})$, $\Omega_{Ga(Sb)}(\vec{r})$, $\Omega_{Ga(As)}(\vec{r})$, $\Omega_{In(Sb)}(\vec{r})$

(8 ions x 5 parameters/ion + 3 offsets) = 43 parameters
guess of potential + interface bond weightings + Temp. dependent segregation

- Method (2) : Superimposed "Bulk" EPM = SEPM

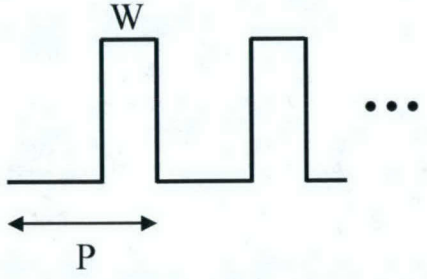
$$V_W(\vec{r}) = \sum_{\vec{g}} V_{\vec{g}}^{W} e^{i\vec{g}\cdot\vec{r}}$$

$$V_B(\vec{r}) = \sum_{\vec{g}} V_{\vec{g}}^{B} e^{i\vec{g}\cdot\vec{r}}$$

$$V(\vec{r}) = rect\left(\frac{z}{W}\right) \cdot V_W(\vec{r}) + \left[1 - rect\left(\frac{z}{W}\right)\right] \cdot V_B(\vec{r})$$

in which:

$$rect\left(\frac{z}{W}\right) = \sum_{n=-M}^{M} \frac{1}{\pi} \sin\left(\frac{\pi W}{P} \cdot n\right) e^{i\frac{2\pi n}{P}z} =$$



Key Point: This construction only requires $V_{\vec{g}}^{W}$ *and* $V_{\vec{g}}^{B}$ *(finite number of form factors)*

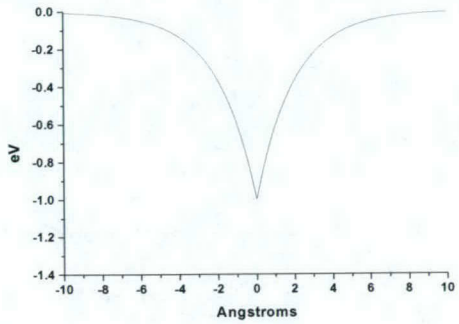
that fit the bulk band diagram plus the offset.

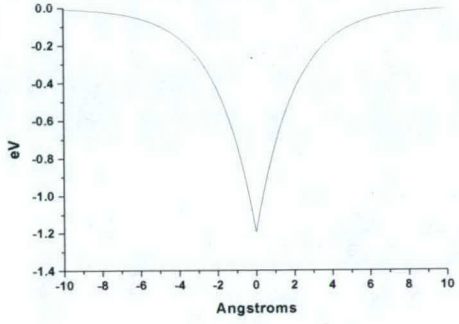
(8 parameters for strained InAs + 7 parameters for GaSb + offset) = 16 parameters

Graphical comparison in 1-dimension

(6ML / 12ML)

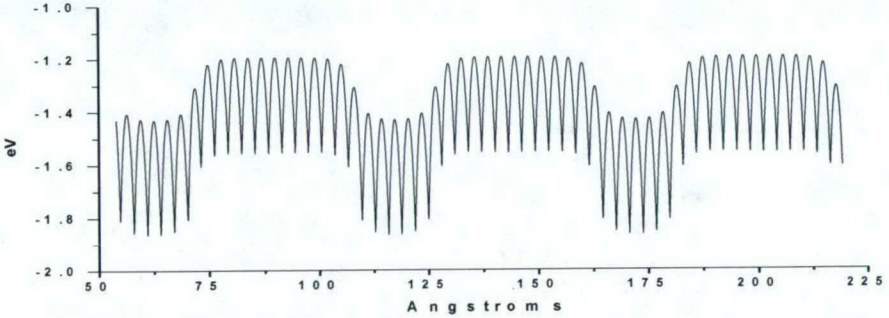
Barrier Lattice Potential





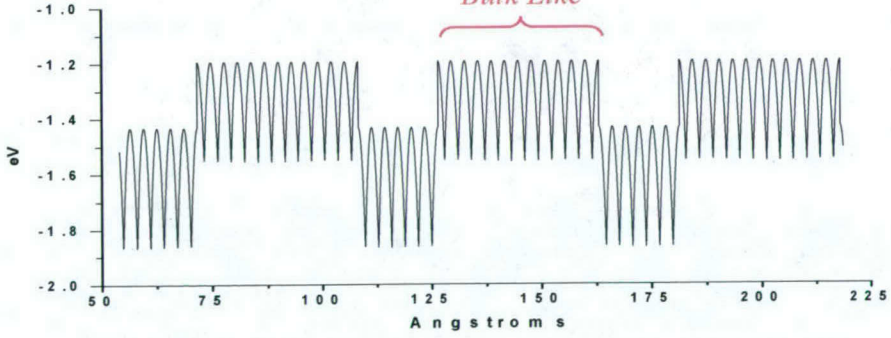
Well Lattice Potential

Method (1) AEPM



Construction requires full knowledge of $V_W(\vec{k})$ *and* $V_B(\vec{k})$ *for* $-Max < \vec{k} < Max$.

Method (2) SEPM



Construction uses finite number of form factors, $V_W(\vec{g})$ *and* $V_B(\vec{g})$.
Interface complexity is covered by one parameter: *Offset*

- For both methods, the final potential can be written as a sum

$$V(\vec{r}) \equiv \sum_{\vec{g}_{\parallel},n} \overline{V}_{\vec{g}_{\parallel},n}\, e^{i(g_x x+g_y y)}\, e^{i\frac{2\pi n}{P}z}$$

SEPM *or* AEPM

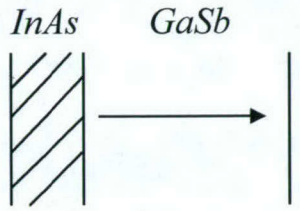
but Fourier coefficients $\overline{V}$ change.

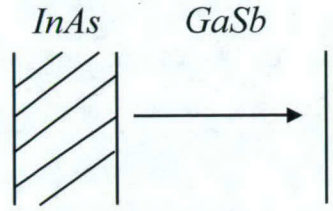
- The Schroedinger Equation for the superlattice is:

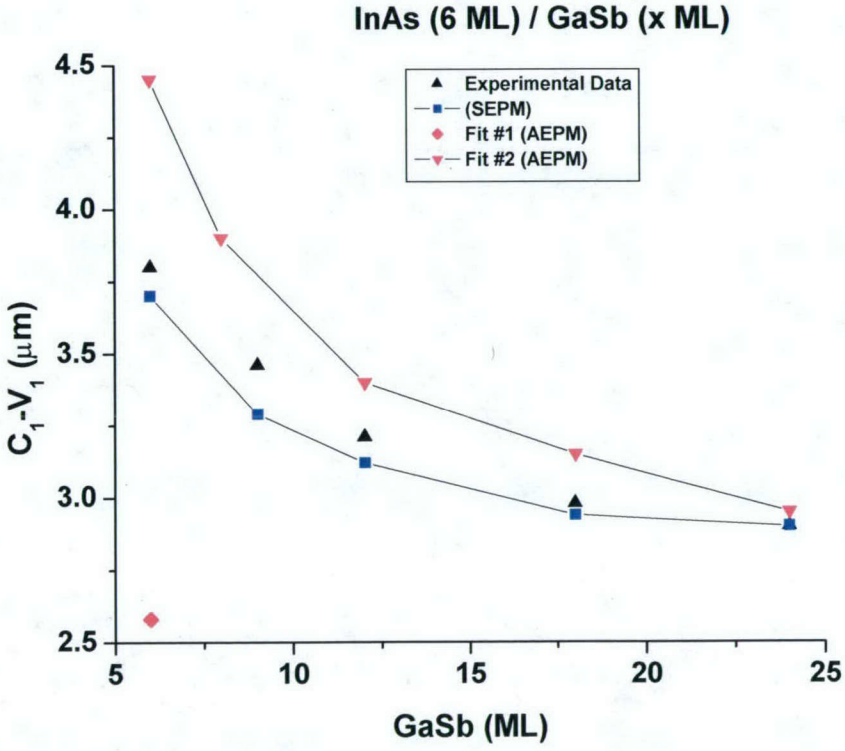
$$\frac{\hbar^2}{2m}\left[\left|\vec{g}_{\parallel}+\vec{\xi}_{\parallel}\right|^2+\left(\frac{2\pi n}{P}+\xi_z\right)^2\right]a_{\vec{g}_{\parallel},n}+\sum_{\vec{g}_{\parallel}',n'}\overline{V}_{\vec{g}_{\parallel}-\vec{g}_{\parallel}',n-n'}\,a_{\vec{g}_{\parallel}',n'}=E(\vec{\xi})\,a_{\vec{g}_{\parallel},n}$$

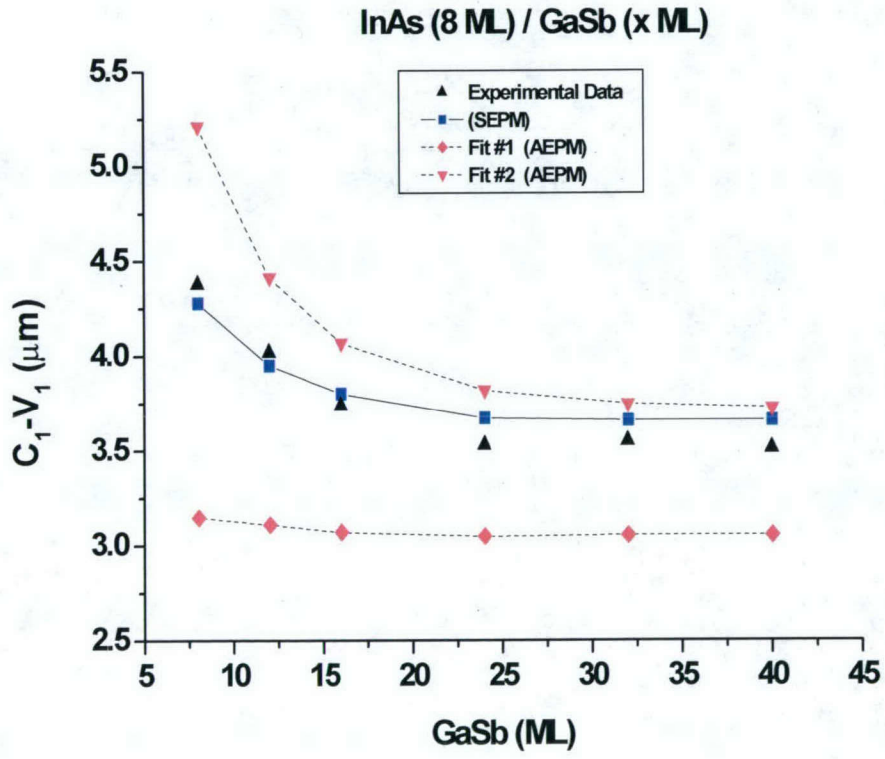
Question for Discussion: ***Which model, SEPM or AEPM, represents reality?***

Superlattice (InAs / GaSb)
Blue Shift Results -vs- GaSb Thickness









- Fit #1 and Fit #2 both provide excellent fits to the *InAs* and *GaSb* band diagrams, but they interpolate differently.

Application of SEPM to Mid-IR Laser Tuning

SEPM model calculations, assuming 24 Å of $In_{0.4}Ga_{0.6}Sb$ hole well and thick $In_{0.2}Ga_{0.8}AsSb$ internal absorbers.